

PATENT
Docket No.: 57953/1221 (ZHA01-01)

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicants	:	Zhang et al.)	
Serial No.	:	10/825,186)	Examiner:
Cnfrm. No.	:	8260)	Marjorie A. Moran
Filing Date	:	April 16, 2004)	Art Unit:
For	:	A METHOD FOR INTRODUCING)	1631
		CONJUGATED CAPS ONTO MOLECULAR)	
		FRAGMENTS AND SYSTEMS AND)	
		METHODS FOR USING THE SAME TO)	
		DETERMINE INTER-MOLECULAR)	
		INTERACTION ENERGIES)	

REQUEST FOR CORRECTED FILING RECEIPT

Mail Stop Amendment
Commissioner for Patents
P.O. Box 1450
Alexandria, VA 22313-1450

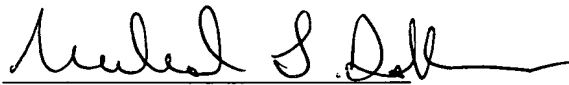
Dear Sir:

Applicants hereby request a corrected filing receipt for the above-identified application. The correct title should be: "A METHOD FOR INTRODUCING CONJUGATED CAPS ONTO MOLECULAR FRAGMENTS AND SYSTEMS AND METHODS FOR USING THE SAME TO DETERMINE INTER-MOLECULAR INTERACTION ENERGIES" (correction underlined). Applicants also enclose an amendment requesting correction of the title on page 1 of the present application in order to make that portion of this application consistent with how the title is set forth elsewhere.

Since Applicants are responsible for this error, the Commissioner is hereby authorized to charge any necessary fees to Deposit Account No. 14-1138. A duplicate copy of this sheet is enclosed.

Respectfully submitted,

Dated: December 12, 2006



Michael L. Goldman
Registration No. 30,727

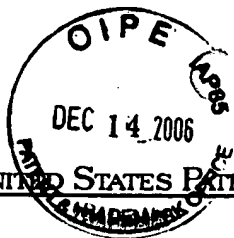
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CERTIFICATE OF MAILING OR TRANSMISSION [37 CFR 1.8(a)]

I hereby certify that this correspondence is being deposited with the United States Postal Service on the date shown below with sufficient postage as first class mail in an envelope addressed to: Mail Stop Amendment, Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450.

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APPL NO.	FILING OR 371 (c) DATE	ART UNIT	FIL FEE REC'D	ATTY. DOCKET NO	DRAWINGS	TOT CLMS	IND CLMS
10/825,186	04/16/2004	1645	709	57953/1221 (ZHA01-01)	24	44	4

Michael L. Goldman
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CONFIRMATION NO. 8260

UPDATED FILING RECEIPT



OC000000014689279

Date Mailed: 12/08/2004

Receipt is acknowledged of this regular Patent Application. It will be considered in its order and you will be notified as to the results of the examination. Be sure to provide the U.S. APPLICATION NUMBER, FILING DATE, NAME OF APPLICANT, and TITLE OF INVENTION when inquiring about this application. Fees transmitted by check or draft are subject to collection. Please verify the accuracy of the data presented on this receipt. If an error is noted on this Filing Receipt, please write to the Office of Initial Patent Examination's Filing Receipt Corrections, facsimile number 703-746-9195. Please provide a copy of this Filing Receipt with the changes noted thereon. If you received a "Notice to File Missing Parts" for this application, please submit any corrections to this Filing Receipt with your reply to the Notice. When the USPTO processes the reply to the Notice, the USPTO will generate another Filing Receipt incorporating the requested corrections (if appropriate).

Applicant(s)

John Zeng Hui Zhang, New York, NY;
Da Wei Zhang, Elmhurst, NY;

Power of Attorney: None

Domestic Priority data as claimed by applicant

This appln claims benefit of 60/463,753 04/17/2003

Foreign Applications

If Required, Foreign Filing License Granted: 06/28/2004

The country code and number of your priority application, to be used for filing abroad under the Paris Convention, is **US10/825,186**

Projected Publication Date: 03/17/2005

Non-Publication Request: No

Early Publication Request: No

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NIXON PEABODY LLP

DEC 10 2004

57953/1221
pkb

**** SMALL ENTITY ******Title**

Method for introducing conjugated caps into molecule fragments and systems and methods for using the same to determine inter-molecular interaction energies

Preliminary Class

435

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Title 35, United States Code, Section 184
Title 37, Code of Federal Regulations, 5.11 & 5.15**

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- 1 -

**A METHOD FOR INTRODUCING CONJUGATED CAPS ONTO
MOLECULAR FRAGMENTS AND SYSTEMS AND METHODS FOR USING
THE SAME TO DETERMINE INTER-MOLECULAR INTERACTION
ENERGIES**

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[0001] This application claims benefit of U.S. Provisional Patent Application
Serial No. 60/463,753, filed April 17, 2003, the disclosure of which is hereby
incorporated by reference in its entirety.

10

FIELD OF THE INVENTION

[0002] This invention relates to a method of introducing conjugated caps onto
molecule fragments. After the molecule portions have been capped, the
intermolecular interaction energy between the decomposed molecule and a second
15 molecule can be calculated using the molecular portions.

BACKGROUND OF THE INVENTION

[0003] A grand challenge in computational chemistry and biology is the
20 accurate quantum mechanical calculation of interaction energies for molecules,
especially larger biological molecules such as proteins. Due to a larger number of
atoms, standard full quantum mechanical or *ab initio* calculation of intermolecular
interaction energy is beyond computational reach. Currently, most theoretical studies
of biological molecules employed classical force fields that are built on pair-wise
25 atomic interaction potentials. Despite the success of classical force field methods in
many applications, they still have significant limitations and quantum mechanical
calculations of interaction energies are often required, e.g., in studying enzyme
reactions.

[0004] Recently, a popular approach to applying quantum mechanical
30 calculation to biological molecules is the hybrid quantum mechanical/molecular
mechanical (QM/MM) approach in which one combines quantum mechanical
methods with molecular force fields for large molecules. In this hybrid QM/MM
approach, one employs quantum mechanical or *ab initio* methods such as Hartree-
Fock (HF) or density functional theory (DFT) methods to treat a small subsystem